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Parallel non-iterative methods for evolutionary semilinear flow problems

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SUMMARY

This paper deals with the efficient numerical solution of semilinear parabolic problems that describe flow phenomena through non-isotropic porous media. For the time integration of such problems, we propose a linearly implicit fractional step method that considers function and operator splittings related to suitable decompositions of the flow domain. The resulting family of elliptic problems is discretized in space by means of the support-operator technique, obtaining a nine-cell finite difference scheme on a logically rectangular grid. Owing to the chosen splittings, the totally discrete scheme involves sets of uncoupled linear systems that can be solved in parallel. Finally, a numerical experiment is included in order to show the unconditionally convergent behaviour of the scheme. Copyright © 2007 John Wiley & Sons, Ltd.

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KEY WORDS: domain decomposition; fractional step method; linearly implicit method; logically rectangular grid; support-operator method

1. INTRODUCTION

The transient state formulation that governs water movement through non-swelling porous media is given by Richards' equation (cf. [1, 2]). If we consider a non-isotropic porous material subject to isothermal conditions, a simplified version of such an equation can be expressed in the form

$$\frac{\partial \psi(\mathbf{x},t)}{\partial t} = \mathbf{div}(K(\mathbf{x})\,\mathbf{grad}\,\psi(\mathbf{x},t)) + g(\psi(\mathbf{x},t)) + f(\mathbf{x},t), \quad (\mathbf{x},t) \in \Omega \times (0,T] \tag{1}$$

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together with suitable initial and boundary conditions. The flow domain $\Omega \subseteq \mathbb{R}^2$ is assumed to be a bounded open set, ψ denotes the pressure head, K is a 2×2 symmetric positive-definite tensor that models hydraulic conductivity, g is a smooth non-linear function that may describe, for instance, root water uptake in soil profiles (cf. [3]) and f is a source/sink term.

In this work, we propose an efficient technique that combines two discretization procedures for the numerical solution of (1). Firstly, Section 2 introduces a linearly implicit fractional step Runge–Kutta method for the time integration. As explained there, the function and operator splittings required by such a method are subordinated to the decomposition of the flow domain into a set of overlapping subdomains. Next, Section 3 handles the spatial discretization, which consists of a finite difference scheme derived from the support-operator method. The new algorithm is formulated for logically rectangular grids, which are naturally involved in the description of certain geometries, e.g. those ones related to flow problems in stratified porous media. In the last section, we include a numerical experiment that illustrates the advantages of the proposed method.

2. TIME SEMIDISCRETIZATION

Let us consider Ω decomposed into the union of m overlapping subdomains, where each one of them consists of a certain number of disjoint connected components, i.e.

$$\Omega = \bigcup_{i=1}^{m} \Omega_i \quad \text{where } \Omega_i = \bigcup_{j=1}^{m_i} \Omega_{ij} \quad \text{such that } \Omega_{ij} \cap \Omega_{ik} = \emptyset \text{ if } j \neq k$$

Next, we define a smooth partition of unity consisting of m functions $\{\rho_i(\mathbf{x})\}_{i=1}^{m}$, where each function $\rho_i : \Omega \to [0,1]$ is defined as follows:

$$\rho_i(\mathbf{x}) = \begin{cases} 0 & \text{if } \mathbf{x} \in \Omega \setminus \Omega_i \\ h_i(\mathbf{x}) & \text{if } \mathbf{x} \in \bigcup\limits_{\substack{j=1 \\ j \neq i}}^{m} (\Omega_i \cap \Omega_j) \\ 1 & \text{if } \mathbf{x} \in \Omega_i \setminus \bigcup\limits_{\substack{j=1 \\ j \neq i}}^{m} (\Omega_i \cap \Omega_j) \end{cases}$$

where

$$0 \leqslant h_i(\mathbf{x}) \leqslant 1 \quad \text{and} \quad \sum_{i=1}^{m} h_i(\mathbf{x}) = 1 \quad \forall\, \mathbf{x} \in \bigcup_{\substack{j=1 \\ j \neq i}}^{m} (\Omega_i \cap \Omega_j)$$

Using this partition of unity, we shall define the following splittings for the spatial differential operator $\mathbf{A}(\mathbf{x}) \equiv \mathbf{div}(K(\mathbf{x})\,\mathbf{grad})$ and function $f(\mathbf{x}, t)$ (cf. [4])

$$\begin{aligned} \mathbf{A}(\mathbf{x}) &= \sum_{i=1}^{m} \mathbf{A}_i(\mathbf{x}) \quad \text{where } \mathbf{A}_i(\mathbf{x}) \equiv \mathbf{div}(K_i(\mathbf{x})\,\mathbf{grad}) \quad \text{and} \quad K_i(\mathbf{x}) \equiv \rho_i(\mathbf{x}) K(\mathbf{x}) \\ f(\mathbf{x}, t) &= \sum_{i=1}^{m} f_i(\mathbf{x}, t) \quad \text{where } f_i(\mathbf{x}, t) \equiv \rho_i(\mathbf{x})\, f(\mathbf{x}, t) \end{aligned} \tag{2}$$

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Note that $K_i(\mathbf{x})$ is also a 2×2 symmetric positive-definite tensor at those points lying on subdomain Ω_i, for every $i\in\{1,2,\ldots,m\}$.

A linearly implicit fractional step Runge–Kutta method with m levels and s internal stages (cf. [5]), considering the splittings given by (2), reduces the original semilinear parabolic problem (1) to the following set of linear elliptic problems, one per internal stage:

$$\begin{cases} \psi_n^k(\mathbf{x}) = \psi_n(\mathbf{x}) + \tau\displaystyle\sum_{\ell=1}^{k} a_{k\ell}^{i_\ell}(\mathbf{A}_{i_\ell}(\mathbf{x})\,\psi_n^\ell(\mathbf{x}) + f_{i_\ell}(\mathbf{x}, t_n + c_\ell\tau)) \\ \qquad\qquad + \tau\displaystyle\sum_{\ell=1}^{k-1} a_{k\ell}^{m+1} g(\psi_n^\ell(\mathbf{x})) \quad \text{for } k=1,2,\ldots,s \\ \psi_{n+1}(\mathbf{x}) = \psi_n(\mathbf{x}) + \tau\displaystyle\sum_{\ell=1}^{s} b_\ell^{i_\ell}(\mathbf{A}_{i_\ell}(\mathbf{x})\,\psi_n^\ell(\mathbf{x}) + f_{i_\ell}(\mathbf{x}, t_n + c_\ell\tau)) + \tau\sum_{\ell=1}^{s} b_\ell^{m+1} g(\psi_n^\ell(\mathbf{x})) \end{cases} \tag{3}$$

for $n=0,1,2,\ldots,N_T$, where $N_T\equiv[T/\tau]-1$ and $i_\ell\in\{1,2,\ldots,m\}$ for every $\ell\in\{1,2,\ldots,s\}$. The semidiscrete solution $\psi_{n+1}(\mathbf{x})$ approximates $\psi(\mathbf{x},t_{n+1})$, where $t_{n+1}=(n+1)\,\tau$ and τ denotes the constant time step. Finally, coefficients $a_{k\ell}^i$, b_k^i and c_k, for $1\leqslant\ell\leqslant k\leqslant s$ and $i\in\{1,2,\ldots,m+1\}$, depend on the chosen method.

3. SPATIAL DISCRETIZATION AND TOTALLY DISCRETE SCHEME

The totally discrete scheme is deduced from the time semidiscrete scheme (3) by using a finite difference spatial discretization based on the support-operator method. Such a method, initially developed in [6] and subsequently discussed in [7], provides a methodology for constructing discrete analogs of invariant first-order differential operators that appear in Equation (1) (i.e. divergence and gradient).

Let us first discretize Ω by means of a logically rectangular grid, whose structure is indexed as follows: if N_x and N_y are positive integers, then the (i,j)-node is given by its coordinates $(x_{i,j}, y_{i,j})$, for $1\leqslant i\leqslant N_x$ and $1\leqslant j\leqslant N_y$. Henceforth, h denotes the spatial mesh size. The spatial discretization used here considers cell-centred approximations for $\psi_n(\mathbf{x})$, $\psi_n^k(\mathbf{x})$, $g(\psi_n^k(\mathbf{x}))$ and $f_i(\mathbf{x},t_n)$ given by $\psi_{n,h}$, $\psi_{n,h}^k$, $g_h(\psi_{n,h}^k)$ and $f_{i,h}(t_n)$, respectively, where $k\in\{1,2,\ldots,s\}$ and $i\in\{1,2,\ldots,m\}$. On the other hand, we consider nodal discretizations for vector functions $\mathbf{w}_n(\mathbf{x})\equiv(w_n^x(\mathbf{x}), w_n^y(\mathbf{x}))$ and nodal evaluations for tensors $K_i(\mathbf{x})$ by means of $\mathbf{w}_{n,h}\equiv(w_{n,h}^x, w_{n,h}^y)$ and $K_{i,h}$, respectively, where $i\in\{1,2,\ldots,m\}$.

For this approximation scheme, it is natural to use the divergence as the first-order *prime operator* (cf. [8]). Based on the invariant definition of the divergence, we can derive a discrete analog $\mathbf{div}_h$ of $\mathbf{div}$ in such a way that, for $i=1,2,\ldots,N_x-1$ and $j=1,2,\ldots,N_y-1$, we obtain the following expression for a discrete vector $\mathbf{w}_{n,h}$:

$$\begin{aligned}(\mathbf{div}_h\,\mathbf{w}_{n,h})_{i,j} = {} & ((w_{i+1,j+1}^x - w_{i,j}^x)(y_{i,j+1} - y_{i+1,j}) - (w_{i,j+1}^x - w_{i+1,j}^x)(y_{i+1,j+1} - y_{i,j}) \\ & - (w_{i+1,j+1}^y - w_{i,j}^y)(x_{i,j+1} - x_{i+1,j}) - (w_{i,j+1}^y - w_{i+1,j}^y)(x_{i+1,j+1} - x_{i,j}))/(2\sigma_{i,j})\end{aligned}$$

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where $w^z_{i,j}$ is the (i,j)th component of $w^z_{n,h}$ that approximates $w^z_n(x_{i,j}, y_{i,j})$ for $z=x, y$; $\sigma_{i,j}$ denotes the area of cell (i,j), whose corresponding nodes are (i,j), $(i+1,j)$, $(i,j+1)$ and $(i+1,j+1)$. Taking into account a discrete approximation of the Gauss' theorem, together with the expression of $\mathbf{div}_h$, we shall construct the *derived operator* $\mathbf{grad}_h$ as the discrete analog of **grad** as follows:

$$(\mathbf{grad}^x_h \psi_{n,h})_{i,j} = ((y_{i,j+1}-y_{i+1,j})\psi_{i,j}+(y_{i-1,j}-y_{i,j+1})\psi_{i-1,j} + (y_{i+1,j}-y_{i,j-1})\psi_{i,j-1}+(y_{i,j-1}-y_{i-1,j})\psi_{i-1,j-1})/(2\eta_{i,j})$$

for $i=2,\ldots,N_x-1$ and $j=2,\ldots,N_y-1$, where $\eta_{i,j}=0.25\,(\sigma_{i,j}+\sigma_{i-1,j}+\sigma_{i,j-1}+\sigma_{i-1,j-1})$ and $\psi_{i,j}$ is the (i,j)th component of $\psi_{n,h}$ that approximates $\psi_n(x_{i,j}, y_{i,j})$. A similar expression holds for $(\mathbf{grad}^y_h \psi_{n,h})_{i,j}$.

Next, by considering the discrete tensors $K_{i,h}$, it is immediate to obtain a finite difference discretization of the second-order elliptic operators $\mathbf{A}_i(\mathbf{x})$. The resulting discrete operators $\mathbf{A}_{i,h} \equiv \mathbf{div}_h(K_{i,h}\,\mathbf{grad}_h)$, for $i \in \{1,2,\ldots,m\}$, are symmetric matrices that involve a local nine-cell stencil. Thus, the totally discrete scheme admits the following formulation:

$$\begin{cases} \psi^k_{n,h} = \psi_{n,h} + \tau \sum_{\ell=1}^{k} a^{i_\ell}_{k\ell}(\mathbf{A}_{i_\ell,h}\,\psi^\ell_{n,h} + f_{i_\ell,h}(t_n + c_\ell \tau)) \\ \qquad\qquad + \tau \sum_{\ell=1}^{k-1} a^{m+1}_{k\ell}\, g_h(\psi^\ell_{n,h}) \quad \text{for } k=1,2,\ldots,s \\ \psi_{n+1,h} = \psi_{n,h} + \tau \sum_{\ell=1}^{s} b^{i_\ell}_{\ell}(\mathbf{A}_{i_\ell,h}\,\psi^\ell_{n,h} + f_{i_\ell,h}(t_n + c_\ell \tau)) + \tau \sum_{\ell=1}^{s} b^{m+1}_{\ell}\, g_h(\psi^\ell_{n,h}) \end{cases} \tag{4}$$

for $n=0,1,2,\ldots,N_T$, where $i_\ell \in \{1,2,\ldots,m\}$ for every $\ell \in \{1,2,\ldots,s\}$.

Taking into account the type of splitting (2) considered in the previous section, the linear system obtained at each internal stage involves the unknowns lying just on one of the subdomains $\{\Omega_i\}_{i=1}^m$. Moreover, since each subdomain Ω_i comprises m_i disjoint connected components, this system can be immediately decomposed into m_i uncoupled subsystems that can be solved in parallel. A remarkable advantage of this technique, compared with classical domain decomposition methods, is that no Schwarz iterations are involved in (4).

4. NUMERICAL EXPERIMENT

In this section we test the behaviour of the numerical algorithm on pseudo-random grids. A similar test is shown in [9] for the classical implicit Euler scheme, combined with the support-operator technique, in the solution of a class of simpler linear parabolic problems.

Let us consider an equation of type (1) posed on $\Omega \times (0,T] \equiv \{\mathbf{x}=(x,y) \in \mathbb{R}^2 : 0<x<1,\ 0<y<1\} \times (0, 0.01]$. Tensor $K(\mathbf{x})$ is defined as $K(\mathbf{x}) = R(\theta) D(\mathbf{x}) R(\theta)^{\mathrm{T}}$, where $R(\theta)$ is a 2×2 rotation matrix with angle $\theta = 5\pi/12$ and $D(\mathbf{x})$ is a 2×2 diagonal matrix whose diagonal entries are $1+2x^2+y^2$ and $1+x^2+2y^2$. The non-linear function is chosen to be $g(\psi) = 1/(1+\psi^3)$, whereas the source/sink term f and both initial and Dirichlet boundary conditions are defined in such a way that $\psi(x,y,t) = \mathrm{e}^{-2\pi^2 t}\sin(\pi x)\sin(\pi y)$ is the exact solution of the problem.

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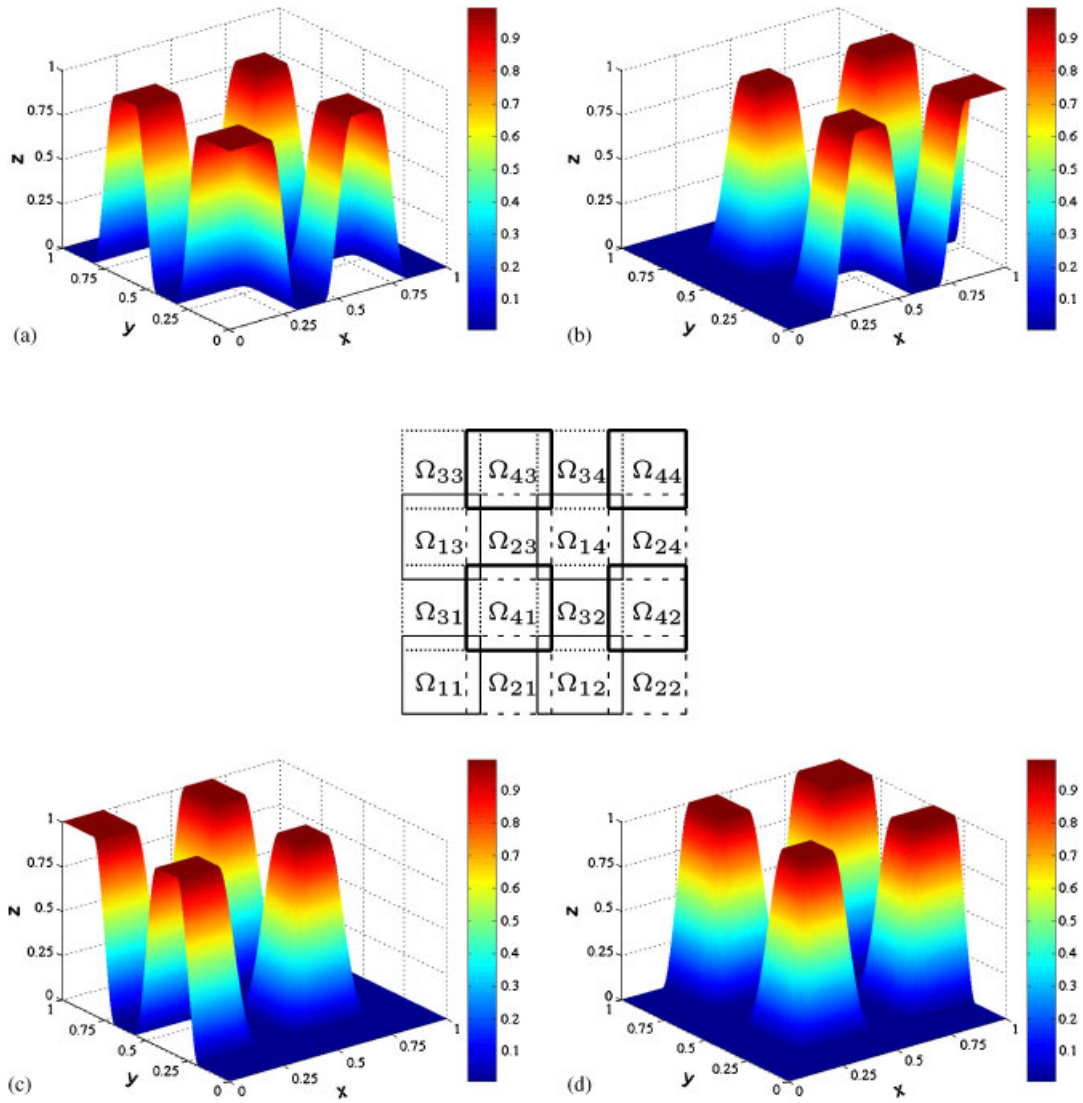

Figure 1. Decomposition of Ω in $m=4$ overlapping subdomains (central plot) and corresponding functions $\rho_i(x,y)$, for $i=1,2,3,4$ (corner plots): (a) $\rho_1(x,y)$; (b) $\rho_2(x,y)$; (c) $\rho_3(x,y)$; and (d) $\rho_4(x,y)$.

We consider a decomposition of Ω in $m=4$ overlapping subdomains, each of which consists of $m_i=4$ disjoint connected components, for $i=1,2,3,4$ (see Figure 1, central plot). On the other hand, piecewise functions $\{\rho_i(\mathbf{x})\}_{i=1}^m$ are defined at the overlapping regions by means of suitable exponential functions that give rise to a $\mathscr{C}^\infty$ partition of unity (see Figure 1, corner plots).

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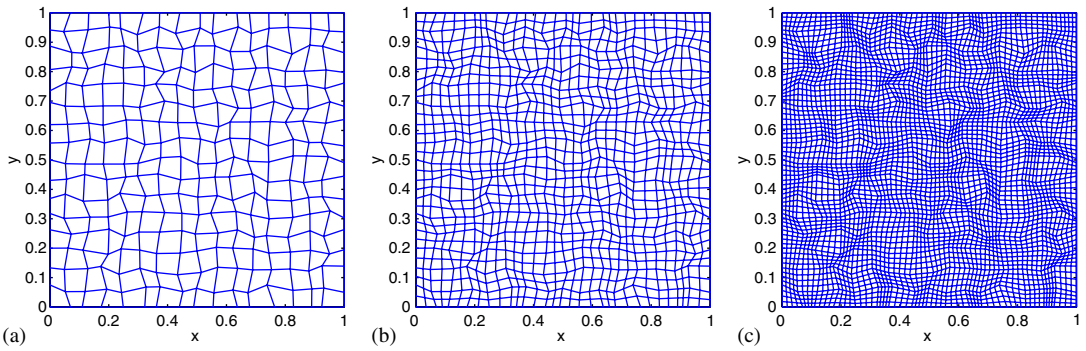

Figure 2. Logically rectangular grids used in the numerical experiment (a) $N=17$; (b) $N=33$; (c) $N=65$.

Next, we use a linearly implicit variant of the fractional implicit Euler method, with four levels ($m=4$) and four stages ($s=4$), for the time integration of our problem. The resulting semidiscrete scheme is, for $n=0,1,2,\ldots,N_T$,

$$\begin{cases} \psi_n^k(\mathbf{x}) = \psi_n(\mathbf{x}) + \tau \sum_{\ell=1}^{k} (\mathbf{A}_\ell(\mathbf{x})\,\psi_n^\ell(\mathbf{x}) + f_\ell(\mathbf{x}, t_{n+1})) + \tau\, g(\psi_n(\mathbf{x})) \quad \text{for } k=1,2,3,4 \\ \psi_{n+1}(\mathbf{x}) = \psi_n^4(\mathbf{x}) \end{cases}$$

The spatial discretization is based on the finite difference method described in Section 3. For this purpose, the flow domain Ω is first discretized by means of a pseudo-random logically rectangular grid $\Omega_N \equiv \{(x_{i,j}, y_{i,j})\}_{i,j=1}^{N}$ with coordinates $x_{i,j}=(i-1)\,h-0.25\,h+0.5\,h\,R_x$ and $y_{i,j}=(j-1)h-0.25h+0.5hR_y$, where $h=1/(N-1)$ and R_x, R_y are pseudo-random numbers generated on the interval $(0,1)$. Figure 2(a) shows an example of such type of grids for $N=17$. In order to study the asymptotic behaviour of the error, we successively refine the original pseudo-random grid by using the following procedure: starting from a given grid, we add the lines that connect, on each cell, the centres of the opposite sides. Figures 2(b) and (c) show the first two refinements for the grid on Figure 2(a).

The combination of the previous discretization procedures gives rise to a totally discrete scheme whose solution is given by the vector $\psi_{n,h} \in \mathbb{R}^{(N-1)\times(N-1)}$, for $n=1,2,\ldots,N_T+1$. The components of $\psi_{n,h}$ are approximations to the exact solution $\psi(\mathbf{x}, t_n)$ at the cell centres of Ω_h. Owing to the domain decomposition splitting considered for $\mathbf{A}(\mathbf{x})$, the linear system obtained at each internal stage reduces to a set of four smaller uncoupled subsystems that can be easily solved in parallel. Therefore, the number of unknowns involved in the computation will decrease from $(N-1)\times(N-1)$ to a number between $n_1\times n_1$ and $n_2\times n_2$, where $n_1=(N-1)(1/4+d)$ and $n_2=(N-1)(1/4+2d)$. For this example, the width of the overlapping regions is assumed to be $2d$, taking $d=\frac{1}{16}$. From a practical point of view, as the amount of available processors increases, each subdomain can be decomposed into a greater number of disjoint components in order to reduce the actual execution time.

Finally, we include two tables that contain the global errors (upper row) and numerical orders of convergence (lower row), obtained for different values of N and τ when using the maximum

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Table I. Global errors and numerical orders of convergence in time for $N=129$ and $\tau_0=10^{-3}$.

τ	τ_0	$\tau_0/2$	$\tau_0/4$	$\tau_0/8$	$\tau_0/16$	$\tau_0/32$
$\|\cdot\|_{L^\infty(0,T;L^2(\Omega))}$	$3.430E-2$	$2.066E-2$	$1.178E-2$	$6.497E-3$	$3.498E-3$	$1.847E-3$
p_2	0.7315	0.8103	0.8582	0.8932	0.9213	—

Table II. Global errors and numerical orders of convergence in space for $\tau=10^{-7}$.

N	17	33	65	129	257
$\|\cdot\|_{L^\infty(0,T;L^2(\Omega))}$	$4.639E-3$	$1.911E-3$	$4.650E-4$	$1.158E-4$	$2.893E-5$
p_2	1.2795	2.0390	2.0056	2.0010	—

norm in time and the L^2-norm in space. The method shows unconditional convergence of first order in time (see Table I) and second order in space (see Table II).

5. CONCLUDING REMARKS

This work describes and numerically tests a new efficient discretization method for the solution of semilinear transient flow problems through non-isotropic porous media of general geometry. Our proposal, which is based on an overlapping domain decomposition technique using a smooth partition of unity, reduces the original problem to the solution of various sets of parallelizable linear systems. As a difference with respect to existing domain decomposition methods, artificial boundary conditions are not imposed on each subdomain and, hence, no Schwarz iterative procedures are needed in the computation. Moreover, regarding other classical approaches (e.g. the combination of a Runge–Kutta method with standard spatial discretization schemes), we obtain an efficient algorithm that explicitly handles non-linear reaction terms and is naturally adapted to non-Cartesian geometries, showing both unconditional convergence and a significant reduction in the actual execution time.

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